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Laboratory Measurements of $3 \rightarrow 2$ X-ray Emission Lines of Ne-like Ni

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ABSTRACT

The intensity ratios between $3 \rightarrow 2$ emission lines in Ni XIX were measured on the Livermore electron beam ion trap (EBIT-I) with a flat-field grating spectrometer and the NASA/GSFC X-ray microcalorimeter. The results are consistent with earlier measurements of Fe XVII and other Ne-like ions at Livermore, and confirm the problems in the atomic modeling of the direct collisional excitation for Ne-like systems.

Subject headings: atomic data — atomic processes — line: formation — X-rays: general

1. INTRODUCTION

Ne-like ions have important spectral diagnostic utilities. Due to their closed shell nature, they are often the most abundant charge states in plasmas with wide temperature ranges. The spectra of Ne-like systems are dominated by the six $3 \rightarrow 2$ lines, including three $3d \rightarrow 2p$ and three $3s \rightarrow 2p$ transitions. Such lines from Fe XVII have been routinely observed in the sun (Parkinson 1975; McKenzie et al. 1980; Phillips et al. 1999), and more recently, in other astronomical sources studied by the grating spectrometers on board *Chandra* and *XMM-Newton* observatories (Canizares et al. 2000; Brinkman et al. 2000; Behar et al. 2001; Raassen et al. 2002; Xu et al. 2002). However, despite the relatively simple atomic level structure of Ne-like ions, it has been known for some time that there are systematic discrepancies between the theoretical predictions of $3 \rightarrow 2$ line intensities and both the astrophysical observations and laboratory measurements (Brown et al. 1998, 2001; Beiersdorfer et al. 2002). The intensity ratio of the two strongest $3d \rightarrow 2p$ lines, commonly known as 3C and 3D (3C/3D), is overpredicted in theory, while the ratio of the $3s \rightarrow 2p$ to $3d \rightarrow 2p$ intensities is underpredicted.

In systematic measurements of the 3C/3D ratio along the Ne-like isoelectronic sequence, Brown et al. (2001) and Beiersdorfer et al. (2001) found that the discrepancy is common to all Ne-like ions. The detailed studies of $3s \rightarrow 2p/3d \rightarrow 2p$ ratio have been limited to Fe XVII so far. Two mutually inconsistent measurements exist for this ratio. Firstly, using the National Institute of Standards and Technology (NIST) electron beam ion trap, Laming et al. (2000) determined that the ratio for Fe XVII was in good agreement with the calculations. Subsequently, using the Livermore EBIT-II electron beam ion trap and the Princeton PLT tokamak, Beiersdorfer et al. (2002; 2003) showed that the ratio was significantly larger than the theoretical predictions. In this paper, we report the results of measurements of Ne-like Ni XIX, and confirm the problems with the theoretical calculations of these line ratios.

2. MEASUREMENT AND ANALYSIS

The present measurement was carried out on the EBIT-I electron beam ion trap at the Lawrence Livermore National Laboratory, employing two types of X-ray spectrometers, i.e, a 44.3m flat-field grating spectrometer and the Goddard X-ray calorimeter developed for the Astro-E2 mission. The Astro-E2 X-ray calorimeter represents the next-generation microcalorimeter replacing the calorimeter from the Astro-E mission installed on EBIT-II in 2000 (Porter et al. 2000). Similarly, the 44.3m grating spectrometer replaces a 5m instrument used earlier (Utter et al. 1999). The resolving power of the grating spectrometer is about 500 and the calorimeter has a FWHM of a little less than 6 eV in the 12–15 Å wavelength band (∼825–1035 eV), which covers the $3 \rightarrow 2$ transitions of Ne-like Ni. All six lines, located at 12.43 (3C), 12.65 (3D), 12.81 (3E), 13.78 (3G), 14.03 (3F), and 14.07 Å (M2), are simultaneously observed with the two instruments.

Because the $3s \rightarrow 2p$ lines are widely separated from the $3d \rightarrow 2p$ lines, it is important that the response functions of the spectrometers are taken into account in the analysis. For the X-ray calorimeter, we used the nominal thickness of various foils separating EBIT-I and the detector to calculate the transmission efficiencies. The grating reflectivity is difficult to model directly and the potential build-up of ice in front of the calorimeter detector may cause the calculated response function to be inaccurate. In order to gauge such effects, we took calibration spectra of various H-like and He-like ions, and used the theoretical intensities of their Rydberg series to verify the spectrometer efficiencies. For the grating spectrometer, H-like and He-like Ne and F were used. For the calorimeter, we also recorded the Rydberg series of O and N, which are particularly sensitive to any ice build-up, should any build-up occur. The theoretical intensities of H-like and He-like lines are calculated with the Flexible Atomic Code (Gu 2003), which is also used to calculate the Ni XIX line intensities in the analysis. These calibration spectra verify the calculated response for the calorimeter, and that the grating response is essentially flat in the 12–15 Å wavelength band.

The measurements for Ni XIX were taken at five electron beam energies. These energies are 1.04, 1.14, 1.24, 1.33, and 1.44 keV, after correcting for the space charge effects of the beam, which we measured by looking for the threshold energies of the $3s \rightarrow 2p$ lines. The energies are all below the ionization threshold of Ni XIX, and no contamination from higher charge states is possible. The energies are also high enough so that no significant Ni XVIII satellite lines were detected. The typical spectra taken at 1.44 keV with the two spectrometers are shown in Figures 1 and 2.

Lines excited by an electron beam are linearly polarized and anisotropic. The measured line intensities must take into account the corrections due to the anisotropic factors. We calculated these correction factors with the Flexible Atomic Code, and obtained the polarization values very similar to those of Ne-like Fe (Zhang et al. 1990). The polarization values of 3C and 3D are about 0.40 with little energy dependence. That of 3E varies from -0.4 to -0.15 at beam energies between 1.0 and 1.5 keV. 3F and 3G have very small polarizations of about 0.05, while that of M2 is about -0.12, all with little energy dependence in the range of interest. The correction factor for the $3s \rightarrow 2p$/3C ratio is about 1.15, while that for the 3E/3C ratio varies from 1.2 to 1.3 in the energy range of interest. No correction is needed for 3D/3C ratio, since the two lines have essentially the same polarization.

In Figure 3, we plot the 3D/3C, 3E/3C, and (3F+3G+M2)/3C ratios of Ni XIX as functions of the beam energy. The error bars represent combined statistical and systematic uncertainties associated with each instrument. Statistics contribute little to the total uncertainties in the 3D/3C and $3s \rightarrow 2p$/3C ratios (<1%). For the 3E/3C ratios, the statistical uncertainties are about 8%. However, the exact line profiles are not known and it is rather difficult to estimate the local background accurately. We estimate the systematic errors associated with these factors by performing fits with different line shapes and varying polynomial approximations to the background. For the 3D/3C and $3s \rightarrow 2p$/3C, such errors are estimated to be 8%, while the errors for 3E/3C ratio are 15% for the grating spectrometer and 20% for the calorimeter due to its lower resolution. The uncertainties due to the polarization corrections of the 3E/3C and $3s \rightarrow 2p$/3C ratios are common to both instruments, and are estimated to be 7%. The uncertainties in these correction factors reflect the errors associated with the theoretical polarization values as well as the depolarization effects of the thermal component of the beam energy, which varies from 110 to 200 eV (Beiersdorfer et al. 1992; Beiersdorfer & Slater 2001). We also included 12% uncertainties for the $3s \rightarrow 2p$/3C ratios, and 3% for the 3E,3D/3C ratios due to the spectrometer response corrections. Overall, the total uncertainties in the measured $3s \rightarrow 2p$/3C ratios are about 16% for both the calorimeter and the grating spectrometer. The uncertainties in the 3D/3C ratios are 9%. The uncertainties in the 3E/3C ratios are 19% for the grating spectrometer and 23% for the calorimeter.

In Figure 3, we also show the comparisons between the measured ratios and various theoretical predictions. We carried out a detailed calculation of Ni XIX line intensities using the Flexible Atomic Code (Gu 2003). In our atomic model, we included electron direct excitation to levels with principle quantum number $n \leq 10$, and resonance excitation contributions to the $n = 3$ manifold, which is treated in the independent-process, isolated-resonance approximation. Resonances of $3lnl'$ type with $n \leq 45$ and $4lnl'$ type with $n \leq 20$ were included in the calculation. These resonances enhance the $3s \rightarrow 2p$/3C and 3E/3C ratios significantly at energies below 1.3 keV, while they have little effect on the 3D/3C ratio. The line ratios obtained with the astrophysical plasma emission code (APEC, version 1.3.1) are also shown (Smith et al. 2001). These ratios are calculated for thermal plasmas with temperatures between 500 and 1000 eV (i.e., an energy of 1 keV in the figure corresponds to a temperature of 500 eV). APEC line intensities do not include resonance excitation contributions.

3. DISCUSSION

The measured 3D/3C ratios in the present work are consistent with those of Brown et al. (2001), which have a value of 0.45 ± 0.05 with little energy dependence. This is about 15% higher than the theoretical prediction of 0.39 calculated with the Flexible Atomic Code. The corresponding ratios calculated by Zhang et al. (1989) and Hibbert et al. (1993) are 0.35. However, these values do not account for the cascade contributions, which are included in the present calculation, and enhances the ratio by about 7%. Therefore, all calculations agree with each other to within 5%, and are about 15-20% lower than the measurement. The measured 3E/3C ratios are about 20–30% higher than the theoretical predictions.

The experimental $3s \rightarrow 2p$/3C ratios are similarly about 20% larger than the theoretical predictions even if the resonance excitation and radiative cascades are taken into account, and the discrepancy persists in the energy region where resonances are expected to be negligible. This is in complete agreement with the similar measurement on Fe XVII by Beiersdorfer et al. (2002), but disagrees with the conclusions of Laming et al. (2000).

The similarly sized discrepancies between the theoretical and experimental line ratios involving 3C suggest that the direct excitation rates for 3C is most likely the problem, as also discussed by Beiersdorfer et al. (2003). Brown et al. (Private Communications) have recently measured the line excitation cross sections of the $3 \rightarrow 2$ transitions in Fe

XVII by normalizing the line intensities to the radiative recombination emission at the Livermore electron beam ion traps, and found that the theoretical 3C cross section is overestimated. In an attempt to understand the origin of this overestimation, we carried out a detailed calculation of the $3 \rightarrow 2$ line excitation rates of both Ni XIX and Fe XVII using a progressively larger configuration interaction basis. Our base model is that used above, and only includes configuration interaction within the $2l^8$ and $2l^7 3l$ manifolds. The next seven models are constructed by adding more configuration complexes to the interaction basis one at a time. These additional configuration complexes are $2l^7 4l'$, $2l^7 5l'$, $2l^7 6l'$, $2l^7 7l'$, $2l^6 3l'^2$, $2l^6 3l' 4l''$, and $2l^5 3l'^3$. The calculated line excitation rates of 3C, 3D, and $3s \rightarrow 2p$ of Ni XIX are shown in Figure 4 as functions of the model size. It is seen that the 3C intensity decreases by about 5% from the base model to the largest model, the $3s \rightarrow 2p$ intensity decreases by about 2%, and the 3D intensity remains unchanged. Clearly, with more configuration interaction, the theoretical line ratios might approach the experimental ratios, but they do so very slowly. However, configuration interaction models are not very effective in addressing the correlations involving highly excited valence orbitals. Better scattering models, such as the close-coupling approximation, are also unlikely to help, since the problem seems to be purely atomic structure related in nature. Many-body perturbation theory (MBPT) may be a more suitable method in this respect. Unfortunately, to the best of our knowledge, there are no existing MBPT calculations of collisional excitation for highly charged Ne-like ions, or even energy levels and oscillator strengths for that matter. If the problem is indeed due to the electron correlations, it should also manifest itself in the calculated oscillator strength for the 3C line. An accurate determination of the radiative decay rate for the upper level of 3C, either through MBPT calculations or experiments, would clearly help to identify the root problem.

The line ratios from APEC are much smaller than both the experimental values and the present theoretical predictions. The discrepancy in the $3s \rightarrow 2p$/3C ratio is understandable, since APEC does not include resonance excitation contributions. However, the disagreement in 3D/3C and 3E/3C ratios indicates that the Ni XIX line emissivities in APEC are not very accurate.

4. CONCLUSION

We measured line ratios between $3 \rightarrow 2$ transitions of Ni XIX using the LLNL electron beam ion trap EBIT-I. The experimental ratios in the present work are consistent with earlier measurements of Fe XVII using the Livermore electron beam ion traps (Brown et al. 1998, 2001; Beiersdorfer et al. 2002) and the PLT tokamak (Beiersdorfer et al. 2001, 2003). All ratios involving 3C as the denominator are about 15-20% higher than various theoretical calculations. We also investigated the effects of configuration interaction on these line ratios, and found that enlarging the interaction basis makes the theoretical values agree with the experiment slightly better. However, configuration interaction approximation is not very effective in treating electron correlation effects involving highly excited orbitals, which we suggest is the main source of the discrepancy. We also compared our measured and calculated ratios with the values obtained from the APEC database. We found that the accuracy of the APEC line ratios are much worse than the theoretical atomic data used in this paper.

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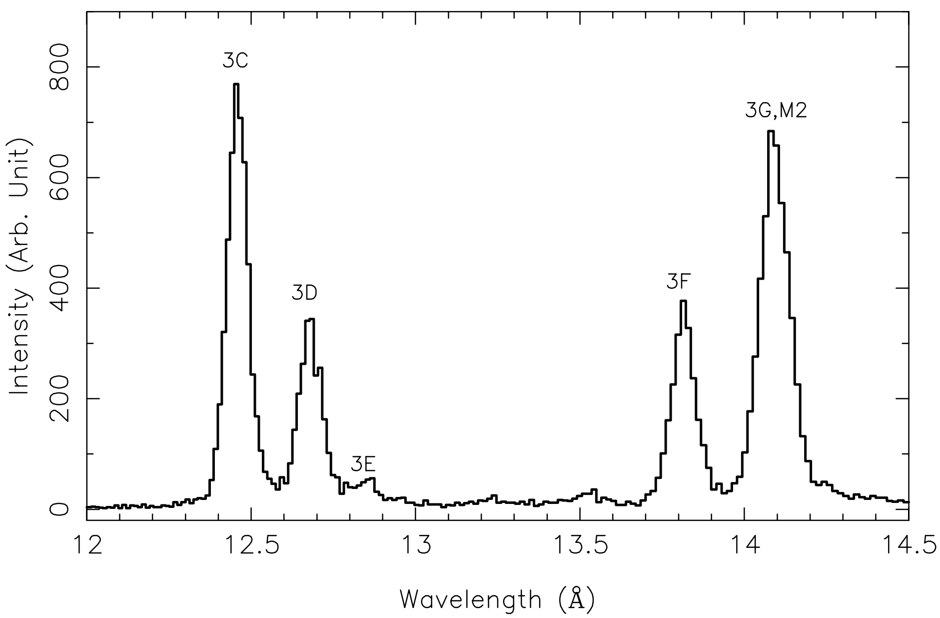

Fig. 1.— Ni XIX spectrum at 1.44 keV taken by the X-ray calorimeter.

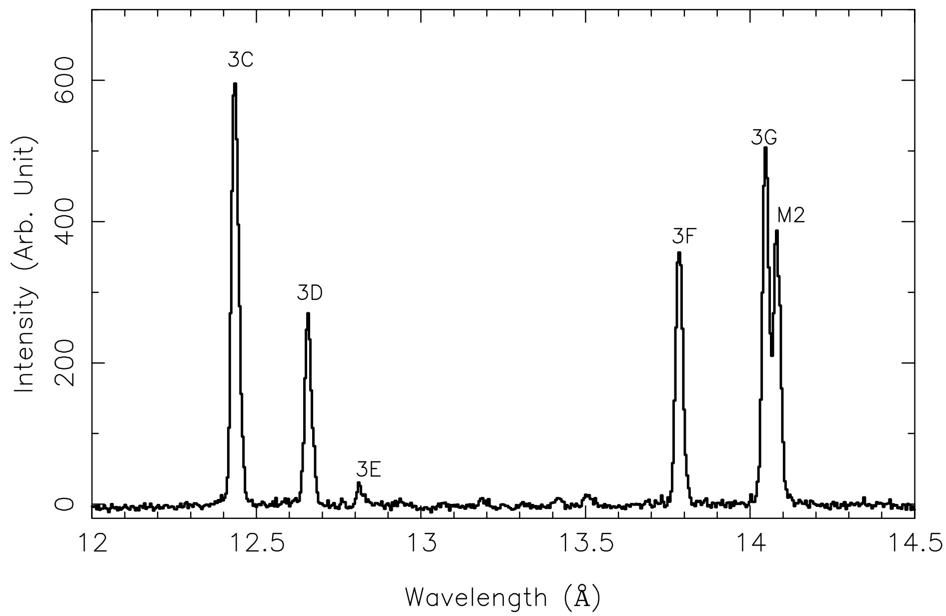

Fig. 2.— Ni XIX spectrum at 1.44 keV taken by the grating spectrometer. A constant background has been subtracted.

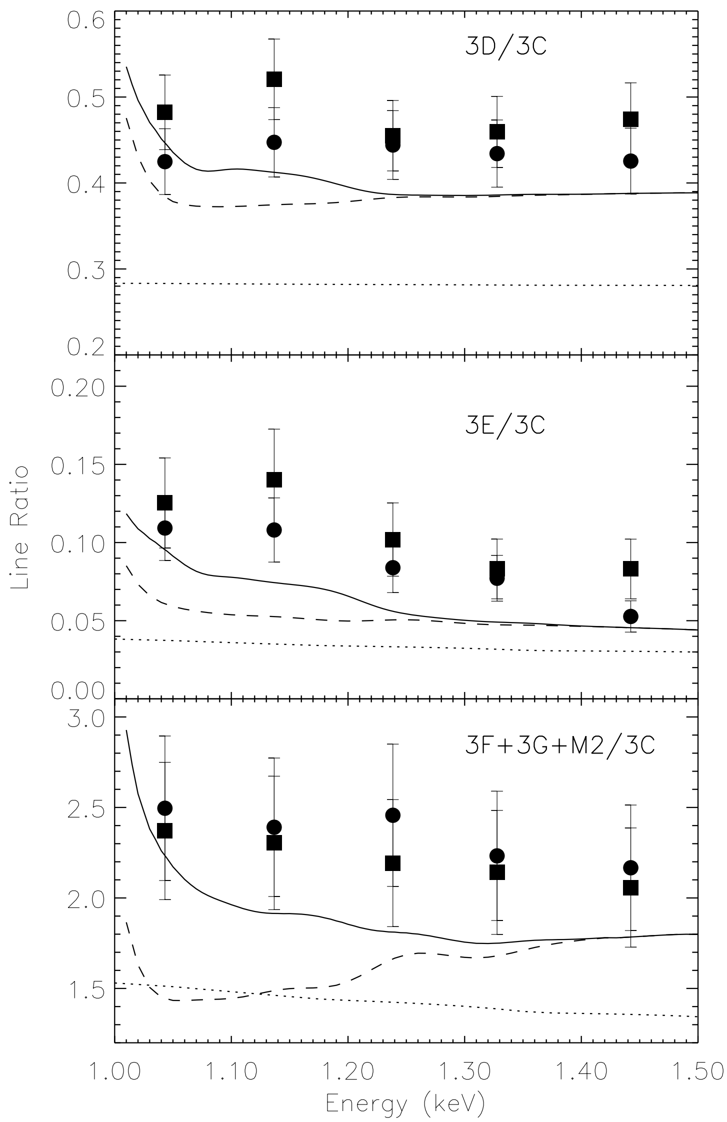

Fig. 3.— The Comparison of the experimental and theoretical Ni XIX line ratios. The filled circles are measurements from the grating spectrometer and the filled squares are those from the X-ray calorimeter. The solid lines are the theoretical calculations using the Flexible Atomic Code, which includes resonance excitation. The dashed lines are the values without resonance excitation. The dotted lines are the ratios from astrophysical plasma emission code (APEC, version 1.3.1), which are for Maxwellian plasmas with temperatures in the 500–1000 eV range (i.e., an energy of 1 keV in the figure corresponds to a temperature of 500 eV).

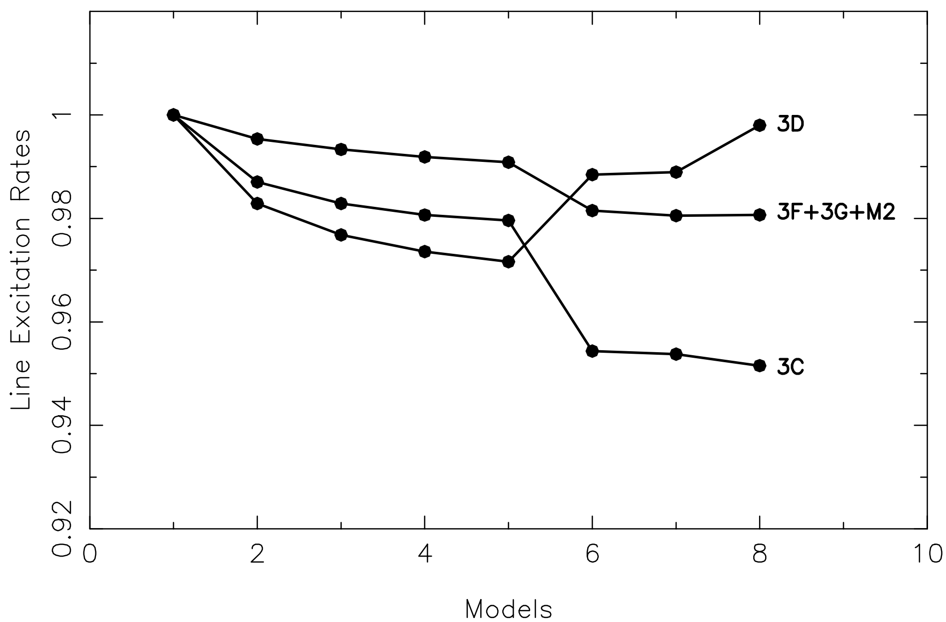

Fig. 4.— Ni XIX 3C, 3D, and $3s \rightarrow 2p$ line excitation rates as functions of the basis size for configuration interaction. Excitation rates are normalized to the values of the base model, which only includes the configuration interactions within $2l^8$ and $2l^7 3l'$ complexes.